Recursive Diagonalization of Quantum Hamiltonians to all order in $\hbar$

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We present a diagonalization method for generic matrix valued Hamiltonians based on a formal expansion in power of $\hbar$. Considering $\hbar$ as a running parameter, a differential equation connecting two diagonalization processes for two very close values of $\hbar$ is derived. The integration of this differential equation allows the recursive determination of the series expansion in powers of $\hbar$ for the diagonalized Hamiltonian. This approach results in effective Hamiltonians with Berry phase corrections of higher order in $\hbar$, and deepens previous works on the semiclassical diagonalization of quantum Hamiltonians which led notably to the discovery of the intrinsic spin Hall effect. As physical applications we consider spinning massless particles in isotropic inhomogeneous media and show that both the energy and the velocity get quantum corrections of order $\hbar^2$. We also derive formally to all order in $\hbar$ the energy spectrum and the equations of motion of Bloch electrons in an external electric field.

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I. INTRODUCTION

Recently, a lot of works have shown the relevance of the Berry phase in semiclassical Physics. For instance, a new set of semiclassical equations of motion including a Berry phase correction was derived within a Lagrangian formalism to account for the adiabatic wave-packet evolution of an electron in an electromagnetic field [1] (see also [2]). A similar semiclassical Lagrangian approach for a light wave-packet in a inhomogeneous medium predicted an optical Hall effect [3]. However this Lagrangian formalism, although adapted to the evolution of a wave-packet, is only semi-classical by construction so that higher order quantum corrections are out of reach. Moreover, it was found that the subsequent derivation of the Hamiltonian presents some difficulties due to the presence of Berry-phase terms [4].

The second difficulty has been solved by a diagonalization procedure with accuracy $\hbar$ for a generic matrix valued Hamiltonian [5]. This method results in an effective semiclassical diagonal Hamiltonian with Berry phase corrections as well as noncommutative covariant coordinates and momentum operators. The resulting generic equations of motion are also corrected by Berry phase terms. In the case of a Bloch electron in electromagnetic field [5][6], this approach leads to the same equations of motion and the same magnetization as in [1]. Therefore, the semiclassical diagonalization of the quantum Hamiltonian not only shows that there is no trouble with the Hamiltonian in the presence of Berry phase terms, but also presents a practical short-cut to derive an effective Hamiltonian, noncommutative coordinates, momentum operators and equations of motion with Berry phase corrections. Moreover, this formalism, which in our opinion, better reflects the physical origin of the phenomena under consideration, is a general one that has been and could still be applied to several other systems in condensed matter or particle physics.

For instance, for spinning particles, this approach led to the discovery of the intrinsic spin Hall effect or topological spin transport. Indeed it was already known that Berry phases, which are in fact spin-orbit couplings, modify semiclassical dynamics of spinning particles in electric [7] and magnetic field [8] as well as in semiconductor [9]. In this last case, the Berry phase in momentum space might be responsible for a transverse dissipationless spin-current in the presence of an electric field. In addition to that, spin-orbit contributions to the propagation of light in isotropic inhomogeneous media has been the focus of several other works [7][10] and has led to a generalization of geometric optics called geometric spinoptics [11].

The diagonalization method of [5] allows to extend these studies to spinning particles interacting with static gravitational fields and goes beyond previous approaches [12][13]. It led to the discovery of new couplings between the spin and magneto-torsion fields which could reveal an hypothetical torsion of space [14][15].

Therefore, the diagonalization procedure of general quantum Hamiltonian has the advantage, compared to the semiclassical wave-packet Lagrangian approach, to gather several different systems into one general scheme. We find particularly interesting that our approach also gives to photons and electrons an equal footing. Indeed the spin Hall effect which offers promising applications both in spintronics and in spinoptics, has its origin, within our formalism, in the noncommutativity of the coordinates for both particles. From this point of view it is always legitimate to wonder whether an electronic phenomenon has its photonic counterpart.

However, the diagonalization procedure mentioned above, despite its advantages, is limited to the semi classical level. It is thus legitimate to wonder about the possibility to go one step further, i.e. to find higher order quantum

corrections. The goal of the present article is to show how to go beyond the semiclassical approximation, a task beyond the reach of the Lagrangian formalism mentioned previously. The method we develop here is entirely new and different from the semiclassical diagonalization of [5], although based on it. It results in an effective diagonal Hamiltonian with Berry phase corrections as well as noncommutative coordinates and momentum operators (in the adiabatic approximation) all written as series expansions in $\hbar$.

More precisely, we propose a procedure to diagonalize recursively in power series of $\hbar$ a generic matrix valued Hamiltonian. The key element of this method relies on considering $\hbar$ as a running parameter. It allows to derive a differential equation connecting two diagonalization processes for two very close values of $\hbar$. The recursive diagonalization can then be obtained by integrating this differential equation order by order in $\hbar$. While this method does not allow an exact derivation of the diagonalized Hamiltonian, it has nevertheless the advantage to make formally possible the computation of quantum corrections of order higher than $\hbar$ (at least second order). To show this point and explain practically our technique, we study as a first example, a photon in an isotropic inhomogeneous medium at the second order in $\hbar$, giving thus corrections to the semi classical equation we derived in [14]. An important consequence of this computation is that the light velocity and the photon energy get a quantum correction of order $\hbar^2$. As a second different physical application, we also provide, formally to all order in $\hbar$, the energy spectrum and the equations of motion for Bloch electrons in a constant external electric field. We show that the equations of motion are formally the same to all order in $\hbar$, and that only the Berry connections get contributions in this expansion.

The paper is organized as follows. In the next section we develop our formalism in the case of a generic matrix valued Hamiltonian. We derive the recursive differential equation in $\hbar$ for the diagonalized Hamiltonian. In section 3 we discuss the semiclassical approximation and derive the generic equations of motion with Berry phases corrections. Section 4 is devoted to exemplify the method beyond the semiclassical level for physically relevant systems. Section 5 is for the conclusion.

II. RECURSIVE DIAGONALIZATION OF QUANTUM HAMILTONIAN

In this section we consider a quantum mechanical system whose state space is a tensor product $L^2\left(\mathcal{R}^3\right) \otimes V$ with V some internal space. In other words, the Hamiltonian of this system can be written as a matrix $H_0\left(\mathbf{P}, \mathbf{R}\right)$ of size $\dim V$ whose elements are operators depending on a couple of canonical variables P and R, the archetype example beeing the Dirac Hamiltonian with $V = C^4$. Our goal is to describe a diagonalization process for this matrix valued quantum Hamiltonian $H_0\left(\mathbf{P}, \mathbf{R}\right)$ recursively as a series expansion in powers of $\hbar$. This expansion in powers of $\hbar$ gives the quantum corrections to the diagonalized Hamiltonian with respect to the classical situation $\hbar = 0$. For example, the first order correction in $\hbar$ corresponds to the semiclassical approximation. Let us stress at this point that, by diagonalization, we always mean here a unitary transformation setting the Hamiltonian in a diagonal matrix form, the diagonal elements beeing operators depending on P and R. That is, we do not aim at finding the eigenvalues, but rather to derive the diagonal representation of Hamiltonians, that are usually relevant for the dynamics.

We will derive the $\hbar$ expansion recursively in the following way. The Planck constant $\hbar$ is formally promoted to a dynamical parameter α in order to establish a differential equation connecting the two diagonalized Hamiltonians at $\hbar = \alpha$ and $\hbar = \alpha + d\alpha$. The integration of this differential equation allows then the recursive determination of the different terms in the expansion of the diagonalized Hamiltonian in powers of α.

A. Set up

To start with, consider a quantum mechanical system with canonical variables $\mathbf{P}$ and $\mathbf{R}$, where $\mathbf{P}$ is the generator of translations. It could be the usual momentum, or the magnetic translation operator of electrons in magnetic Bloch bands in solid state physics as discussed in the section devoted to the physical applications (see also [6]).

Let consider the commutator between the canonical variables as a dynamical parameter α, that is

$$[\mathbf{P}, \mathbf{R}] = -i\alpha \tag{1}$$

Consider now the three following assumptions :

1. The Hamiltonian of the system can be written as a matrix of a certain size $H_0\left(\mathbf{P}, \mathbf{R}\right)$, that is a matrix whose coefficients depend on $\mathbf{P}$ and $\mathbf{R}$. The typical example is the free Dirac Hamiltonian (a 4×4 matrix), but as shown in [5] an electron in a periodic potential also fits in this set up.

2. Assume moreover, that for each value of α, $H_0\left(\mathbf{P}, \mathbf{R}\right)$ is exactly diagonalized through a matrix $U_\alpha(\mathbf{P}, \mathbf{R})$, i.e.

$$U_\alpha\left(\mathbf{P}, \mathbf{R}\right) H_0\left(\mathbf{P}, \mathbf{R}\right) U_\alpha^+\left(\mathbf{P}, \mathbf{R}\right) = \varepsilon_\alpha\left(\mathbf{P}, \mathbf{R}\right) \text{ if } [\mathbf{P}, \mathbf{R}] = -i\alpha \tag{2}$$

where $\varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)$ is a diagonal matrix.

The index in $U_\alpha(\mathbf{P},\mathbf{R})$ underlines the fact that the diagonalization matrix depends a-priori on α since the diagonalization process involves recombination of powers of $\mathbf{P}$ and $\mathbf{R}$, and thus involves commutators of these variables (see [5]).

3. The diagonalization is known when $\alpha = 0$, that is when $\mathbf{P}$ and $\mathbf{R}$ commute. This assumption is crucial, since it allow to start a recursive diagonalization process in powers of α. This last assumption has also the advantage to be quite reasonable, since in many cases, the diagonalization is very easy to perform when $[\mathbf{P},\mathbf{R}] = 0$. Actually, in this case the Hamiltonian can be seen as depending only on $\mathbf{P}$ for example, $\mathbf{R}$ being an external parameter. More about this point can be found in [5].

B. The differential equation

1. α as a parameter

We will now consider α as a running parameter in order to find a relation between $\varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)$ and $\varepsilon_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right)$. But to facilitate the computation of $\varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)$ as explained in [5], we first need to write the Hamiltonian as well as all expressions involving the canonical operators $\mathbf{R}$ and $\mathbf{P}$, in a symmetrized form. By this, we mean that whatever the prescription for the arrangement of the canonical variables (full symmetrization for instance or Weyl prescription) in the initial Hamiltonian, one will always rewrite it (and other expressions too) in a form where all the powers of $\mathbf{P}$ have been put half on the left and half of the right of the expression. Of course this symmetrization will introduce terms of order α due to the commutation relations. Note again that this is just a convention which facilitates the diagonalization.

To start with, consider the diagonalization at the scale α

$$U_\alpha\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_\alpha^+\left(\mathbf{P},\mathbf{R}\right) = \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)\ \text{if}\ [\mathbf{P},\mathbf{R}] = -i\alpha \tag{3}$$

and similarly for $\alpha + d\alpha$.

$$U_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right)H_0\left(\mathbf{P},\mathbf{R}\right)U_{\alpha+d\alpha}^+\left(\mathbf{P},\mathbf{R}\right) = \varepsilon_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right)\ \text{if}\ [\mathbf{P},\mathbf{R}] = -i\left(\alpha+d\alpha\right) \tag{4}$$

Let us develop this last relation to the first order in $d\alpha$,

$$\varepsilon_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right) = U_\alpha H_0 U_\alpha^+ + d\alpha\left(\partial_\alpha U_\alpha H_0 U_\alpha^+ + U_\alpha H_0 \partial_\alpha U_\alpha^+\right)$$

where for clarity we have omitted the $\mathbf{P}$ and $\mathbf{R}$ dependence in the right hand side (note that here we assume the relation $[\mathbf{P},\mathbf{R}] = -i\left(\alpha+d\alpha\right)$ and not $[\mathbf{P},\mathbf{R}] = -i\alpha$). This latter expression at the first order in $d\alpha$, reduces to

$$\begin{aligned}\varepsilon_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right) &= U_\alpha H_0 U_\alpha^+ + d\alpha\left(\partial_\alpha U_\alpha U_\alpha^+ \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right) + \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)U_\alpha\partial_\alpha U_\alpha^+\right)\\ &= U_\alpha H_0 U_\alpha^+ + \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)\left(\partial_\alpha U_\alpha U_\alpha^+ + U_\alpha\partial_\alpha U_\alpha^+\right)d\alpha + \left[\partial_\alpha U_\alpha U_\alpha^+, \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)\right]d\alpha\end{aligned}$$

This differential equation is the main point of this paper. We now show how to compute explicitly each term of the right hand side, to make it tractable.

2. Computation of $\partial_\alpha U_\alpha\left(\mathbf{P},\mathbf{R}\right)U_\alpha^+\left(\mathbf{P},\mathbf{R}\right) + U_\alpha\left(\mathbf{P},\mathbf{R}\right)\partial_\alpha U_\alpha^+\left(\mathbf{P},\mathbf{R}\right)$

From the equality

$$U_{\alpha+d\alpha}(\mathbf{P},\mathbf{R})U_{\alpha+d\alpha}^+(\mathbf{P},\mathbf{R}) = 1\ \text{when}\ [\mathbf{P},\mathbf{R}] = -i\left(\alpha+d\alpha\right) \tag{5}$$

one obtains

$$d\alpha\left(\partial_\alpha U_\alpha\left(\mathbf{P},\mathbf{R}\right)U_\alpha^+\left(\mathbf{P},\mathbf{R}\right) + U_\alpha\left(\mathbf{P},\mathbf{R}\right)\partial_\alpha U_\alpha^+\left(\mathbf{P},\mathbf{R}\right)\right) = 1 - U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) \tag{6}$$

Note that here $U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) \neq 1$, since $[\mathbf{P},\mathbf{R}] = -i\left(\alpha+d\alpha\right)$. As a consequence, we can ultimately rewrite :

$$\varepsilon_{\alpha+d\alpha}\left(\mathbf{P},\mathbf{R}\right) = U_\alpha H_0 U_\alpha^+ + \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)\left[1 - U_\alpha U_\alpha^+\right] + \left[\partial_\alpha U_\alpha U_\alpha^+, \varepsilon_\alpha\left(\mathbf{P},\mathbf{R}\right)\right]d\alpha \tag{7}$$

we now need to rewrite $U_\alpha H_0 U_\alpha^+$.

3. Computation of $U_\alpha(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R})$ and final form for the differential equation.

Here, the important point to keep in mind is that $[\mathbf{P}, \mathbf{R}] = -i(\alpha + d\alpha)$, so that

$$U_\alpha(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R}) \neq \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \tag{8}$$

To compute $U_\alpha H_0 U_\alpha^+$ we introduce two "fictitious" variables ,$\mathbf{r}, \mathbf{p}$, commuting with $\mathbf{P}$ and $\mathbf{R}$ and such that $[\mathbf{p}, \mathbf{r}] = id\alpha$. We can consider $\mathbf{r}$ and $\mathbf{p}$ as an arbitrary couple of "small" canonical variables each of magnitude $\sqrt{d\alpha}$. As a consequence

$$[\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}] = -i\alpha \tag{9}$$

so that in virtu of Eq.2 we have the equality

$$U_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) H_0(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) U_\alpha^+(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) = \varepsilon_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) \tag{10}$$

since $\mathbf{P} + \mathbf{p}$ and $\mathbf{R} + \mathbf{r}$ form a couple of canonical variables with commutator $-i\alpha$. By the same trick, and for practical purpose, we can write :

$$U_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) U_\alpha^+(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) = 1 \tag{11}$$

As a consequence, using Eqs. 10 and 11 we can rewrite our differential equation Eq. 7 as :

$$
\begin{aligned}
\varepsilon_{\alpha+d\alpha}(\mathbf{P}, \mathbf{R}) =\ & \varepsilon_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) \\
& - U_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) H_0(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) U_\alpha^+(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) - U_\alpha(\mathbf{P}, \mathbf{R}) H_0(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R}) \\
& + \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \left[U_\alpha(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) U_\alpha^+(\mathbf{P} + \mathbf{p}, \mathbf{R} + \mathbf{r}) - U_\alpha(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R}) \right] \\
& + \left[\partial_\alpha U_\alpha(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R}), \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \right] d\alpha
\end{aligned}
$$

Now, we expand the R.H.S to the second order in powers of $\mathbf{p}$ and $\mathbf{r}$. Since those two variables satisfy non trivial commutation relations, we choose to expand the R.H.S. on the basis $p_i, r_i, p_i p_j, r_i r_j, p_i r_j$ for $i \neq j$, and $\frac{p_i r_i + r_i p_i}{2}$ (Birkhoff-Witt factorization theorem). As a consequence, the term $p_i r_i$ or $r_i p_i$ have to be rearranged in combination of $\frac{p_i r_i + r_i p_i}{2}$ and $\frac{p_i r_i - r_i p_i}{2} = \frac{id\alpha}{2}$.

The expansion computation is similar to the one presented in [5] (apart from some minor additional terms), and thus is not reproduced here. We are led to the identification of the zeroth order in $\mathbf{p}, \mathbf{r}$

$$
\begin{aligned}
\varepsilon_{\alpha+d\alpha}(\mathbf{P}, \mathbf{R}) =\ & \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) + \left[\partial_\alpha U_\alpha(\mathbf{P}, \mathbf{R}) U_\alpha^+(\mathbf{P}, \mathbf{R}), \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \right] d\alpha \\
& + \frac{1}{2} \left\{ \mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l} \nabla_{P_l} \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) + \nabla_{P_l} \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \mathcal{A}_\alpha^{P_l} \right\} d\alpha \\
& + \frac{i}{2} \left\{ \left[\varepsilon_\alpha(\mathbf{P}, \mathbf{R}), \mathcal{A}_\alpha^{R_l} \right] \mathcal{A}_\alpha^{P_l} d\alpha - \left[\varepsilon_\alpha(\mathbf{P}, \mathbf{R}), \mathcal{A}_\alpha^{P_l} \right] \mathcal{A}_\alpha^{R_l} - \left[Asym \mathcal{A}_\alpha^{P_l, R_l}, \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \right] \right\} d\alpha \\
& + \frac{id\alpha}{2} \left\{ Asym \left\{ \nabla_{P_l} \nabla_{R_l} \varepsilon_\alpha(\mathbf{P}, \mathbf{R}) \right\} - U_\alpha Asym \left\{ \nabla_{P_l} \nabla_{R_l} H_0(\mathbf{P}, \mathbf{R}) \right\} U_\alpha^+ \right\}
\end{aligned} \tag{12}
$$

where we have defined the Berry phases [5] (note the absence of α in factor compared to the usual definition)

$$
\begin{aligned}
\mathcal{A}_\alpha^{R_l} &= iU_\alpha(\mathbf{P}, \mathbf{R}) \nabla_{P_l} U_\alpha^+(\mathbf{P}, \mathbf{R}) \\
\mathcal{A}_\alpha^{P_l} &= -iU_\alpha(\mathbf{P}, \mathbf{R}) \nabla_{R_l} U_\alpha^+(\mathbf{P}, \mathbf{R})
\end{aligned}
$$

and the "second order" Berry phase

$$\mathcal{A}_\alpha^{P_l, R_l} = \left[\nabla_{R_k} \nabla_{P_l} U_\alpha(\mathbf{P}, \mathbf{R}) \right] U_\alpha^+(\mathbf{P}, \mathbf{R})$$

We have moreover introduced the linear operation $Asym$ [5]. It acts on a symmetrical function in $\mathbf{P}$ and $\mathbf{R}$ in the following way :

$$Asym \left\{ \frac{1}{2} A(\mathbf{R}) B(\mathbf{P}) + \frac{1}{2} B(\mathbf{P}) A(\mathbf{R}) \right\} = [B(\mathbf{P}), A(\mathbf{R})] \tag{13}$$

the functions $A(\mathbf{R})$ and $B(\mathbf{P})$ beeing typically monomials in $\mathbf{R}$ and $\mathbf{P}$ arising in the series expansions of the physical quantities.

Note that the *Asym* operator especially in the term $U_\alpha^+ Asym\{\nabla_{P_l}\nabla_{R_l}H_0(\mathbf{P},\mathbf{R})\}U_\alpha^+$, is not particularly elegant. It could in fact be rewritten as an infinite series of differential operators, but the gain does not seem to be clear at this point. Moreover, in our examples, our choice will appear to be the most convenient.

Ultimately, we arrive at the following differential equation

$$
\begin{aligned}
\frac{d}{d\alpha}\varepsilon_\alpha(\mathbf{P},\mathbf{R}) = & \left[\partial_\alpha U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}),\varepsilon_\alpha(\mathbf{P},\mathbf{R})\right] \\
& + \left\{\frac{1}{2}\mathcal{A}_\alpha^{R_l}\nabla_{R_l}\varepsilon_\alpha(\mathbf{P},\mathbf{R}) + \nabla_{R_l}\varepsilon_\alpha(\mathbf{P},\mathbf{R})\mathcal{A}_\alpha^{R_l} + \mathcal{A}_\alpha^{P_l}\nabla_{P_l}\varepsilon_\alpha(\mathbf{P},\mathbf{R}) + \nabla_{P_l}\varepsilon_\alpha(\mathbf{P},\mathbf{R})\mathcal{A}_\alpha^{P_l}\right\} \\
& + \frac{i}{2}\left\{\left[\varepsilon_\alpha(\mathbf{P},\mathbf{R}),\mathcal{A}_\alpha^{R_l}\right]\mathcal{A}_\alpha^{P_l} - \left[\varepsilon_\alpha(\mathbf{P},\mathbf{R}),\mathcal{A}_\alpha^{P_l}\right]\mathcal{A}_\alpha^{R_l} - \left[Asym\mathcal{A}_\alpha^{P_l,R_l},\varepsilon_\alpha(\mathbf{P},\mathbf{R})\right]\right\} \\
& + \frac{i}{2}\left\{Asym\{\nabla_{P_l}\nabla_{R_l}\varepsilon_\alpha(\mathbf{P},\mathbf{R})\} - U_\alpha Asym\{\nabla_{P_l}\nabla_{R_l}H_0(\mathbf{P},\mathbf{R})\}U_\alpha^+\right\}
\end{aligned}
\tag{14}
$$

To complete the diagonalization process, we have to couple this equation with the evolution as a function of α of the transformation matrix $U_\alpha(\mathbf{P},\mathbf{R})$. To find this last one, let us combine Eqs. 6 and 11 to get

$$
0 = U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) - U_\alpha(\mathbf{P}+\mathbf{p},\mathbf{R}+\mathbf{r})U_\alpha^+(\mathbf{P}+\mathbf{p},\mathbf{R}+\mathbf{r}) + d\alpha\left[\partial_\alpha U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) + U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R})\right]
$$

This latter expression can be, similarly to the energy, expanded as

$$
0 = \partial_\alpha U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) + U_\alpha(\mathbf{P},\mathbf{R})\partial_\alpha U_\alpha^+(\mathbf{P},\mathbf{R}) - \frac{i}{2}Asym\left(\mathcal{A}_\alpha^{P_l,R_l} + \left(\mathcal{A}_\alpha^{P_l,R_l}\right)^+\right) - \frac{i}{2}\left[\mathcal{A}_\alpha^{R_l},\mathcal{A}_\alpha^{P_l}\right]
\tag{15}
$$

With these two equations Eqs. 14 and 15 at hand, our diagonalization process can be performed. Actually, since all quantities are matrix valued and since $\varepsilon_\alpha(\mathbf{P},\mathbf{R})$ is by definition a diagonal matrix, we can separate the energy equation Eq. 14 in a diagonal and a non diagonal part such that we are led to the following two equations

$$
\frac{d}{d\alpha}\varepsilon_\alpha(\mathbf{P},\mathbf{R}) = \mathcal{P}_+[\text{R.H.S. of Eq. 14}]
\tag{16}
$$

$$
0 = \mathcal{P}_-[\text{R.H.S. of Eq. 14}]
\tag{17}
$$

where $\mathcal{P}_+[...]$ and $\mathcal{P}_-[...]$ denote the projection on the diagonal and non-diagonal part respectively. These two equations are supplemented by the differential unitarity condition

$$
0 = \partial_\alpha U_\alpha(\mathbf{P},\mathbf{R})U_\alpha^+(\mathbf{P},\mathbf{R}) + U_\alpha(\mathbf{P},\mathbf{R})\partial_\alpha U_\alpha^+(\mathbf{P},\mathbf{R}) - \frac{i}{2}Asym\left(\mathcal{A}_\alpha^{P_l,R_l} + \left(\mathcal{A}_\alpha^{P_l,R_l}\right)^+\right) - \frac{i}{2}\left[\mathcal{A}_\alpha^{R_l},\mathcal{A}_\alpha^{P_l}\right]
\tag{18}
$$

We claim that those three equations Eqs.16-18 allow to determine recursively in powers of α the energy of the quantum system in question. Actually, the integration over α of Eq. 16 gives $\varepsilon_\alpha(\mathbf{P},\mathbf{R})$ at order n in α when knowing all quantities at order $n-1$. By the same token, Eqs. 17 and 18 (whose meaning is that $U_\alpha(\mathbf{P},\mathbf{R})$ is unitary at each order in α) involve $\partial_\alpha U_\alpha(\mathbf{P},\mathbf{R})$, and allow to recover $U_\alpha(\mathbf{P},\mathbf{R})$ at order n by integration over α. Note however that these two equations allow only fixing partially $U_\alpha(\mathbf{P},\mathbf{R})$, leaving m real parameters free with m the size of the matrix. This reflects a kind of gauge invariance (we will see a practical example of this in section four). Actually, the diagonalization matrix is not unique, so that we are left with some choice of the parameters. For example one can impose the diagonal elements to be real (see below in the example). As a consequence, the diagonalization process is perfectly controlled order by order in the series expansion in α.

III. THE SEMICLASSICAL APPROXIMATION

In this section we consider the Hamiltonian diagonalization at the semiclassical level and the resulting equations of motion. Actually, the semiclassical approximation has recently found new important applications in particle and solid state physics. Notably, the equations of motion reveal a new contribution coming from the Berry curvature. This contribution, called the anomalous velocity, modifies profoundly the dynamics of the particles. For instance, the spin Hall effect of electrons and holes in semiconductors [9], as well as the new discovered optical Hall effect [3][7][10][14] can be interpreted in this context. Similarly, the recent experimental discovery of the monopole in momentum can also be elegantly interpreted as the influence of the Berry curvature on the semiclassical dynamics of Bloch electrons [16][17].

A. The semiclassical energy

The consideration of Eq. 14 alone is sufficient to deduce the semiclassical diagonal Hamiltonian. Indeed, writing $\varepsilon_\alpha = \varepsilon_0 + \alpha\varepsilon_1$, with ε_0 the diagonalized energy at the zero order, Eq. 14 is solved by (putting $\alpha = \hbar$)

$$\varepsilon\left(\mathbf{P},\mathbf{R}\right) \;=\; \varepsilon_0\left(\mathbf{P},\mathbf{R}\right) + \hbar\left\{\frac{1}{2}A_0^{R_l}\nabla_{R_l}\varepsilon_0\left(\mathbf{P},\mathbf{R}\right) + \nabla_{R_l}\varepsilon_0\left(\mathbf{P},\mathbf{R}\right)A_0^{R_l} + A_0^{P_l}\nabla_{P_l}\varepsilon_0\left(\mathbf{P},\mathbf{R}\right)\right.$$

$$\left. + \nabla_{P_l}\varepsilon_0\left(\mathbf{P},\mathbf{R}\right)A_0^{P_l}\right\} + \frac{i\hbar}{2}\mathcal{P}_+\left\{\left[\varepsilon_0\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_0^{R_l}\right]\mathcal{A}_0^{P_l} - \left[\varepsilon_0\left(\mathbf{P},\mathbf{R}\right),\mathcal{A}_0^{P_l}\right]\mathcal{A}_0^{R_l}\right\} \tag{19}$$

where we have introduced the notations $A_0^{\mathbf{R}} = \mathcal{P}_+\left[\mathcal{A}_0^{\mathbf{R}}\right]$ and $A_0^{\mathbf{P}} = \mathcal{P}_+\left[\mathcal{A}_0^{\mathbf{P}}\right]$.

This latter expression can also be written

$$\varepsilon\left(\mathbf{P},\mathbf{R}\right) \simeq \varepsilon\left(\mathbf{p},\mathbf{r}\right) + \frac{i\hbar}{2}\mathcal{P}_+\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_0^{R_l}\right]\mathcal{A}_0^{P_l} - \left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),\mathcal{A}_0^{P_l}\right]\mathcal{A}_0^{R_l}\right] + O(\hbar^2) \tag{20}$$

where we have defined the projected dynamical operators (covariant coordinates and momentum operators)

$$\begin{aligned}\mathbf{r} &= \mathbf{R} + \hbar A_0^{\mathbf{R}}\\ \mathbf{p} &= \mathbf{P} + \hbar A_0^{\mathbf{P}}\end{aligned} \tag{21}$$

with $\mathcal{A}_0^{\mathbf{R}} = i\left[U_0\nabla_{\mathbf{P}}U_0^+\right]$, $\mathcal{A}_0^{\mathbf{P}} = -i\left[U_0\nabla_{\mathbf{R}}U_0^+\right]$, and $\mathcal{A}_0^{\mathbf{P},\mathbf{R}} = \left[\nabla_{\mathbf{R}}\nabla_{\mathbf{P}}U_0\right]U_0^+$.

The matrix $U_0\left(\mathbf{P},\mathbf{R}\right)$ is the diagonalization matrix for H_0 when the operators are supposed to be commuting quantities, the diagonalized energy being $\varepsilon_0\left(\mathbf{P},\mathbf{R}\right)$. When $\mathbf{P}$ and $\mathbf{R}$ do not commute, the matrix $U_0\left(\mathbf{P},\mathbf{R}\right)$ does not diagonalize H_0 anymore. In order to get the corrections to the energy at the semiclassical order due to the noncommutativity of $\mathbf{P}$ and $\mathbf{R}$ we have to compute $\varepsilon_1\left(\mathbf{P},\mathbf{R}\right)$. Note that in Eq. 19, the symmetrization defined above (that is all the powers of $\mathbf{P}$ have been put half on the left and half of the right in each expression) is assumed. From the diagonal Hamiltonian, we can now derive the equations of motion for the covariant operators.

B. The equations of motion

Given the Hamiltonian derived in the previous subsection, the equations of motion can now be easily derived. As usual, the dynamics equations have to be considered, not for the usual position and momentum, but rather for the projected variables $\mathbf{r}$ and $\mathbf{p}$. Actually, these latter naturally appear in our diagonalization process at the $\hbar$ order. Let us remark, as now well known, that their components do not commute any more. Actually (removing the index α for clarity)

$$\begin{aligned}\left[r_i,r_j\right] &= i\hbar^2\Theta_{ij}^{rr} = i\hbar^2\left(\nabla_{P_i}A_{R_j} - \nabla_{P_j}A_{R_i}\right) + \hbar^2\left[A_{R_j},A_{R_i}\right]\\ \left[p_i,p_j\right] &= i\hbar^2\Theta_{ij}^{pp} = -i\hbar^2\left(\nabla_{R_i}A_{P_j} - \nabla_{R_j}A_{P_i}\right) + \hbar^2\left[A_{P_i},A_{P_j}\right]\\ \left[p_i,r_j\right] &= -i\hbar\delta_{ij} + i\hbar^2\Theta_{ij}^{pr} = -i\hbar\delta_{ij} - i\hbar^2\left(\nabla_{R_i}A_{R_j} + \nabla_{P_j}A_{P_i}\right) + \hbar^2\left[A_{P_i},A_{R_j}\right]\end{aligned} \tag{22}$$

the Θ_{ij} being the so called Berry curvatures.

Using now our Hamiltonian yields directly to general equations of motion for $\mathbf{r}$, $\mathbf{p}$:

$$\dot{\mathbf{r}} = \frac{i}{\hbar}\left[\mathbf{r},\varepsilon\left(\mathbf{p},\mathbf{r}\right)\right] + \frac{i}{\hbar}\left[\mathbf{r},\frac{i\hbar}{2}\mathcal{P}_+\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),A_{R_l}\right]A_{P_l} - \left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),A_{P_l}\right]A_{R_l}\right]\right]$$

$$\dot{\mathbf{p}} = \frac{i}{\hbar}\left[\mathbf{p},\varepsilon\left(\mathbf{p},\mathbf{r}\right)\right] + \frac{i}{\hbar}\left[\mathbf{p},\frac{i\hbar}{2}\mathcal{P}_+\left[\left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),A_{R_l}\right]A_{P_l} - \left[\varepsilon\left(\mathbf{p},\mathbf{r}\right),A_{P_l}\right]A_{R_l}\right]\right] \tag{23}$$

The commutators can be computed through the previous commutation rules between $\mathbf{r}$ and $\mathbf{p}$. The last term in each equation represents a contribution of "magnetization" type and has the advantage to present this general form whatever the system initially considered. In the context of Bloch electrons in a magnetic field, it gives exactly the magnetization term revealed in [1] (see [6]). For spinning particles in static gravitational fields, this term gives a coupling between the spin and the intrinsic angular momentum with magneto-torsion fields [14][15]. It is interesting to note that both the Hamiltonian Eq. 20 and the equations of motion have already been derived in article [5] .Our method appears then to be an extension of [5]. However, although relying on this previous method, it seems to us more elegant, and offers to possibility to go beyond the semiclassical level. This will appear very important in the next section to compute the velocity of a spinning massless particle (photon) in an inhomogeneous medium. The second application is the determination of the equations of motion of a Bloch electron in an external constant electric field. In both situations we are going to consider the second order in $\hbar$ quantum effects.

IV. PHYSICAL APPLICATIONS

A. Massless spinning particles in an isotropic inhomogeneous medium.

We consider here the dynamics of a spinning massless particle propagating in a isotropic inhomogeneous medium of index $n(\mathbf{R})$. We thus start with the Hamiltonian of a massless Dirac particle in an curved space of metric $g^{ij}(\mathbf{R}) = n^{-1}(\mathbf{R}) \delta^{ij}$ as in [11][14]. The case of higher spin (like the photon) can be treated in the same manner through the Bargman-Wigner equations as in [14]. For this reason we limit ourself to the Dirac particles (with the convention $c = 1$) and write the Hamiltonian as

$$H_0 = \frac{1}{2}\left(\alpha.\mathbf{P}F(\mathbf{R}) + F(\mathbf{R})\alpha.\mathbf{P}\right) \tag{24}$$

with $F(\mathbf{R}) = n^{-1}(\mathbf{R})$. Let us start to recover the first order diagonalization given in [14]. To exploit the previous general formula we write all quantities as a series expansion in α, thus $\varepsilon_\alpha = \varepsilon_0 + \alpha\varepsilon_1 + ...$, $U_\alpha = U_0 + \alpha U_1 + ...$, $\mathcal{A}_\alpha^R = \mathcal{A}_0^R + \alpha\mathcal{A}_1^R + ...$ and the same for all expressions. In these expressions, all terms are functions of $\mathbf{P}$ and $\mathbf{R}$ and are thus assumed to be symmetrized in the sense defined above.

1. First order (semiclassical) diagonalization.

We already know (see [14]) that at the zeroth order in α, that is when $\mathbf{R}$ and $\mathbf{P}$ commute, the Hamiltonian diagonalization can be performed through the following Foldy-Wouthuysen unitary matrix

$$U_0(\mathbf{P}) = \frac{\sqrt{\mathbf{P}^2} + \beta\widetilde{\alpha}.\mathbf{P}}{\sqrt{2\mathbf{P}^2}} \tag{25}$$

(where β and $\widetilde{\alpha}$ are the usual notations for the "Dirac matrices") such that in the diagonal representation the Hamiltonian becomes

$$U_0 H_0(\mathbf{P}, \mathbf{R}) U_0^+ = \varepsilon_0(\mathbf{P}, \mathbf{R}) = \frac{1}{2}\left(\beta F(\mathbf{R})\sqrt{\mathbf{P}^2} + \beta\sqrt{\mathbf{P}^2}F(\mathbf{R})\right) \tag{26}$$

From the unitary matrix, we can deduce that at this order, only $\mathcal{A}_0^{\mathbf{R}} = i[U\nabla_{\mathbb{P}}U^+]$ is non zero, thus $\mathcal{A}_0^{\mathbf{P}} = -i\hbar[U\nabla_{\mathbf{R}}U^+] = 0 + O(\alpha)$, and $\mathcal{A}_0^{P_l, R_l} = 0 + O(\alpha)$. Obviously, when $\mathbf{P}$ and $\mathbf{R}$ do not commute, the matrix $\varepsilon_0(\mathbf{P}, \mathbf{R})$ does not diagonalize H_0 anymore and one has to go to higher order in the expansion in α.

Let thus consider the diagonalization at order α. The differential equation Eq. 14 at the zeroth order (at this order, we consider only in the right hand side of this equation the terms of order α^0) reduces to

$$\frac{d}{d\alpha}\varepsilon_\alpha(\mathbf{P}, \mathbf{R}) = \frac{1}{2}\left[\mathcal{A}_0^{R_l}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R}) + \nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R})\mathcal{A}_0^{R_l}\right] + \left[U_1(\mathbf{P}, \mathbf{R})U_0^+(\mathbf{P}), \varepsilon_0(\mathbf{P}, \mathbf{R})\right] \tag{27}$$

and can be divided in two parts

$$\frac{d}{d\alpha}\varepsilon_\alpha(\mathbf{P}, \mathbf{R}) = \frac{1}{2}\mathcal{P}_+\left[\mathcal{A}_0^{R_l}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R}) + \nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R})\mathcal{A}_0^{R_l}\right] \tag{28}$$

and

$$0 = \frac{1}{2}\mathcal{P}_-\left[\mathcal{A}_0^{R_l}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R}) + \nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R})\mathcal{A}_0^{R_l}\right] + \left[U_1(\mathbf{P}, \mathbf{R})U_0^+(\mathbf{P}), \varepsilon_0(\mathbf{P}, \mathbf{R})\right] \tag{29}$$

(the last term being always anti-diagonal at this order). By integrating Eq. 28 with respect to α from o to $\hbar$ the first equation, we get the energy operator at the first order in $\alpha = \hbar$ which reads

$$\varepsilon_\alpha(\mathbf{P}, \mathbf{R}) = \varepsilon_0(\mathbf{P}, \mathbf{R}) + \frac{\hbar}{2}A_0^{R_l}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R}) + \frac{\hbar}{2}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R})A_0^{R_l}$$

The energy ε_α can be recombined under the usual form [5][14] and written in term of the covariant coordinate operator $\mathbf{r}^+$ as

$$\varepsilon_\alpha(\mathbf{P}, \mathbf{r}) = \frac{\beta}{2}\left(F(\mathbf{r})\sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2}F(\mathbf{r})\right) \tag{30}$$

with

$$\mathbf{r} = \mathbf{R} + \hbar A_0^{\mathbf{R}} = \mathbf{R} + i\hbar \frac{\mathbf{P} \times \mathbf{\Sigma}}{2\mathbf{P}^2} \tag{31}$$

where $A_0^{\mathbf{R}}$ means that we need only the diagonal part of $\mathcal{A}_0^{\mathbf{R}}$. The matrix $\mathbf{\Sigma} = \mathbf{1} \otimes \sigma$ is a 4×4 matrix.

From the last two equations we can deduce the equations of motion in the semiclassical approximation. Indeed, for a particle of positive energy only $\varepsilon(\mathbf{P}, \mathbf{r}) = \frac{1}{2}\left(F(\mathbf{r})\sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2}F(\mathbf{r})\right)$ with now $\mathbf{r} = \mathbf{R} + i\frac{\mathbf{P} \times \mathbf{S}}{\mathbf{P}^2}$ a 2×2 matrix (the spin matrix is $\mathbf{S} = \hbar\sigma/\mathbf{2}$), the usual relations $\mathbf{r} = -\frac{i}{\hbar}[\mathbf{r}, \varepsilon(\mathbf{P}, \mathbf{r})]$ and $\mathbf{P} = -\frac{i}{\hbar}[\mathbf{P}, \varepsilon(\mathbf{P}, \mathbf{r})]$, lead to the by now well known equations of motion

$$\begin{aligned}
\dot{\mathbf{r}} &= \nabla_{\mathbf{P}}\varepsilon + \hbar\dot{\mathbf{P}} \times \Theta^{rr} \\
\dot{\mathbf{P}} &= \nabla_{\mathbf{r}}\varepsilon
\end{aligned} \tag{32}$$

where $[r_i, r_j] = i\hbar^2\Theta_{ij}^{rr} = i\hbar^2\varepsilon_{ijk}\Theta_k^{rr} = -i\hbar\varepsilon_{ijk}\lambda\frac{P^k}{P^3}$, and $\lambda = \mathbf{S}.\mathbf{P}/P$ the helicity. These latter equations are very important because they induce the optical Hall effect or spin Hall effect of light (for the photon one just has to replace the Pauli matrices σ by the spin one matrices) as a consequence of the anomalous velocity term $\hbar\dot{\mathbf{P}} \times \Theta^{rr}$. This effect has been discussed in several circumstances [3][10] [11] and was considered in a quantum mechanical context in [5][7][14]. From Eq.32 we see that the velocity components are given by the relation

$$v^i = \frac{1}{2}\left(\frac{c}{n(\mathbf{r})}\frac{P^i}{P} + \frac{P^i}{P}\frac{c}{n(\mathbf{r})}\right) + \frac{\lambda}{P^2}\frac{c}{n(\mathbf{r})}\varepsilon_{ijk}P^k\frac{\partial \ln n}{\partial x^i} \tag{33}$$

Note that the symmetrization for the last term was unnecessary due to the presence of the $\hbar$. Symmetrizing would just add $\hbar^2$ corrections.

From the last relation, we deduce the velocity

$$v = \frac{c}{n(\mathbf{r})}\left(1 + \frac{\lambda^2}{P^2}\left((\nabla \ln n)^2 - \frac{1}{P^2}(\mathbf{P}.\nabla \ln n)^2\right)\right)^{1/2} \tag{34}$$

The velocity can be rewritten $v = \frac{c}{n(\mathbf{r})}\left(1 + \frac{\lambda^2}{P^2}(\nabla \ln n)^2 \sin^2 \vartheta\right)^{1/2}$ with ϑ the angle between $\mathbf{P}$ and $\nabla \ln n$. We therefore find the important result that the light velocity in an isotropic inhomogeneous medium does not have the well known expression $v(\mathbf{r}) = c/n(\mathbf{r})$ but has rather quantum corrections due to the spin-orbit couplings when $\mathbf{P}$ and $\nabla \ln n$ are not parallel. However, at this level of approximation, we can not yet conclude regarding the velocity since the quantum corrections are of order $\hbar^2$ which is beyond the first order approximation. To get a clear answer one has to compute the Hamiltonian diagonalization at the second order in $\hbar$.

2. Second order diagonalization

To perform the diagonalization at order α^2 we need to know the transformation matrix U_α at the first order in α, i.e., the matrix $U_1(\mathbf{P}, \mathbf{R})$ (i.e. the Foldy Fouthuysen transformation when $\mathbf{R}$ and $\mathbf{P}$ do not commute). The equation in Eq. 29 allows to find easily the transformation matrix U_α at this order. Indeed, given that at zeroth order

$$\mathcal{P}_-\left[\mathcal{A}_0^{R_l}\nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R}) + \nabla_{R_l}\varepsilon_0(\mathbf{P}, \mathbf{R})\mathcal{A}_0^{R_l}\right] = 0 \tag{35}$$

as a consequence of $\widetilde{\alpha}\beta + \beta\widetilde{\alpha} = 0$, we can write

$$\left[U_1(\mathbf{P}, \mathbf{R})U_0^+(\mathbf{P}), \varepsilon_0(\mathbf{P}, \mathbf{R})\right] = 0 \tag{36}$$

Likewise, the differential unitarity condition Eq. 18 at the same zero order becomes

$$U_1(\mathbf{P}, \mathbf{R})U_0^+(\mathbf{P}) + U_0(\mathbf{P})U_1^+(\mathbf{P}, \mathbf{R}) = 0 \tag{37}$$

We claim that $U_\alpha(\mathbf{P}, \mathbf{R})$, and consequently the Berry phases, are unchanged with respect to the zeroth order. That is the matrix Eq. 25 also diagonalizes H_0 at the first order in α. Indeed, we can easily see with the help of Eqs. 36 37, that the following transformation $\left(1 - \alpha U_1(\mathbf{P}, \mathbf{R})U_0^+(\mathbf{P})\right)U_\alpha(\mathbf{P}, \mathbf{R})$ which at order α is equal to $U_0(\mathbf{P})$ diagonalizes

H_0, e.g. $U_0^+ H_0 U_0 = \varepsilon_0 (\mathbf{P}, \mathbf{R}) + \alpha \varepsilon_1 (\mathbf{P}, \mathbf{R})$ (this is an example of the gauge transformation in the diagonalization matrix we mentioned previously).

As a consequence, the Berry phases do not get any contribution at the first order. Therefore we have $A_\alpha^{\mathbf{P}} = -i\mathcal{P}_+ [U\nabla_{\mathbf{R}} U^+] = 0 + O(\alpha^2)$ implying $A_\alpha^{P_l, R_l} = 0 + O(\alpha^2)$ and also

$$A_\alpha^{\mathbf{R}} = i\hbar \mathcal{P}_+ [U\nabla_P U^+] = i\frac{\mathbf{P} \times \mathbf{\Sigma}}{2\mathbf{P}^2} + O(\alpha^2) \tag{38}$$

Now, to find the second order Hamiltonian we write the differential equation Eq. 14 at the first order.

$$\frac{d}{d\alpha}\varepsilon_\alpha (\mathbf{P}, \mathbf{R}) = \frac{1}{2}\mathcal{P}_+ \left[\mathcal{A}_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) + \nabla_{R_l} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) \mathcal{A}_\alpha^{R_l} \right] + \frac{i}{2} Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) \} \tag{39}$$

since trivially $Asym \{ \nabla_{P_l} \nabla_{R_l} H_0 (\mathbf{P}, \mathbf{R}) \} = 0$. To show how to solve this equation, recall that at the first order $\varepsilon_\alpha (\mathbf{P}, \mathbf{R})$ is given by

$$\varepsilon_\alpha (\mathbf{P}, \mathbf{R}) = \varepsilon_0 (\mathbf{P}, \mathbf{R}) + \frac{\alpha}{2} A_\alpha^{R_l} \nabla_{R_l} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) + \frac{\alpha}{2} \nabla_{R_l} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) A_\alpha^{R_l} \tag{40}$$

(recall that all our expressions are supposed symmetrized in $\mathbf{P}$ and $\mathbf{R}$ as explained in the beginning of the previous section), so that Eq. 39 becomes

$$\begin{aligned} \frac{d}{d\alpha}\varepsilon_\alpha (\mathbf{P}, \mathbf{R}) = & \frac{1}{2} A_\alpha^{R_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) + \frac{1}{2}\nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_l} + \frac{\alpha}{4} A_\alpha^{R_k} A_\alpha^{R_l} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \\ & + \frac{\alpha}{2} A_\alpha^{R_k} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_l} + \frac{\alpha}{4} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_k} A_\alpha^{R_l} + \frac{i}{2} Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \} \end{aligned}$$

and as a result after integration,

$$\begin{aligned} \varepsilon_\alpha (\mathbf{P}, \mathbf{R}) - \varepsilon_0 (\mathbf{P}, \mathbf{R}) = & \frac{\alpha}{2} A_\alpha^{R_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) + \frac{\alpha}{2}\nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_l} + \frac{\alpha^2}{8} A_\alpha^{R_k} A_\alpha^{R_l} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \\ & + \frac{\alpha^2}{4} A_\alpha^{R_k} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_l} + \frac{\alpha^2}{8} \nabla_{R_k} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) A_\alpha^{R_k} A_\alpha^{R_l} \\ & + \frac{i}{2} \int_0^\alpha d\alpha\, Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \} \end{aligned}$$

Given our symmetrization convention, this last expression $\varepsilon_\alpha (\mathbf{P}, \mathbf{R})$ can be shown to be equal to $\varepsilon_0 (\mathbf{P}, \mathbf{r})$.

Given this last result, we can solve our differential equation at the second order approximation. Actually, recalling that $\varepsilon_0 (\mathbf{P}, \mathbf{R}) = \frac{1}{2} \left(\beta F(\mathbf{R})\sqrt{\mathbf{P}^2} + \beta\sqrt{\mathbf{P}^2} F(\mathbf{R}) \right)$, one can first state that :

$$Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \} = \left[\sqrt{\mathbf{P}^2}, F(\mathbf{r}) \right]$$

so that :

$$\frac{i}{2} \int_0^\alpha d\alpha\, Asym \{ \nabla_{P_l} \nabla_{R_l} \varepsilon_0 (\mathbf{P}, \mathbf{R}) \} = -\frac{1}{4}\hbar \left[\sqrt{\mathbf{P}^2}, F(\mathbf{r}) \right]$$

Now, by replacing α by $\hbar$ and projecting on the positive energy subspace, our solution is :.

$$\varepsilon (\mathbf{P}, \mathbf{r}) = \frac{1}{2} \left(F(\mathbf{r})\sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{1}{4}\hbar \left[\sqrt{\mathbf{P}^2}, F(\mathbf{r}) \right]$$

which can be also written

$$\varepsilon (\mathbf{P}, \mathbf{r}) = \frac{1}{2} \left(F(\mathbf{r})\sqrt{\mathbf{P}^2} + \sqrt{\mathbf{P}^2} F(\mathbf{r}) \right) - \frac{1}{4}\frac{\hbar^2}{\sqrt{\mathbf{P}^2}}\mathbf{P}\nabla F(\mathbf{r})$$

(the symmetrization of the last term is not necessary due to the presence of the $\hbar^2$.)

Now, concerning the equation of motion at the second order, their form is only formally identical to Eq. 32. Actually, the energy has been changed by getting quantum corrections of order $\hbar^2$. Moreover, the term $\hbar\dot{\mathbf{P}}\times\Theta^{rr}$ in Eq.32 has to be understood as beeing symetrized between $\mathbf{P}$ and $\mathbf{r}$.

Let us conclude this section by noting from the equations of motion that the speed of light get also quantum correction of order $\hbar^2$. Indeed, one has now a correction to Eq. 33 of order $\hbar^2$ (remember that λ is of order $\hbar$) such that the velocity components become

$$v^i = \frac{1}{2}\left(\frac{c}{n(\mathbf{r})}\frac{P^i}{P} + \frac{P^i}{P}\frac{c}{n(\mathbf{r})}\right) + \frac{\lambda}{2P^2}\varepsilon_{ijk}\left(P^k\frac{\partial \ln n}{\partial x^i}\frac{c}{n(\mathbf{r})} + \frac{\partial \ln n}{\partial x^i}\frac{c}{n(\mathbf{r})}P^k\right) + \frac{\hbar^2}{4}\frac{c}{n(\mathbf{r})}\left(\frac{1}{P}\partial_i \ln n - \frac{P_iP_j}{P^3}\partial_j \ln n\right)$$

Interestingly the corrective term does not give any contribution to the velocity at this order of approximation so that the velocity is indeed given by Eq. 34 at the order $\hbar^2$

$$v = \frac{c}{n(\mathbf{r})}\left(1 + \frac{\lambda^2}{P^2}\left((\nabla \ln n)^2 - \frac{1}{P^2}(\mathbf{P}.\nabla \ln n)^2\right)\right)^{1/2} + O(\hbar^3)$$

It is worth mentioning that in the context of photons propagating in a smoothly inhomogeneous medium we are apparently led to a contradiction with known results. Indeed, it is known from optics that the second order corrections in a smoothly inhomogeneous medium are responsible for the linear birefringence, i.e., the equations of motion depend on the linear polarization of the particle [18] and not only on helicity as found here. One possible explanation of this discrepancy might be that here the photon in an inhomogeneous medium is treated as a quantum particle moving in a static gravitational field, so that the medium index is equivalent to a metric. This approach is perhaps too restrictive since by doing so, we take only into account the geometry and neglect all electrodynamical processes which are relevant for the interpretation of the linear birefringence [18]. In other words, an inhomogeneous medium might be considered to be equivalent to a gravitational field at the semiclassical order only, since the electrodynamics plays a role at the second order. If true, our approach beyond the first order is strictly speaking only valid for spinning particles in a static gravitational field.

B. The electron in a time dependent electric field

As a second example, we consider a spinless non-relativistic electron in a periodic potential submitted to an external time dependent electric field. We limit ourself to this simple case because a second order computation can easily be performed as shown below, and leave more complicated cases with a position dependent electric field and a magnetic field to future works. Because of the non-trivial vacuum configuration, that is the band structure of the energy spectrum in solid state physics this example fits in our formalism similarly to the Dirac equation. Important new results where recently found in the context of Bloch electron. Indeed, the semi-classical equations of motion where found to be modified by Berry phase terms [1][5][6][19], changing profoundly the properties of electron transport in a solid [20]. It is thus interesting to go beyond the semi-classical approximation to check wether new effects might be revealed.

1. First order

Since the initial diagonalization matrix when $\alpha = 0$ is not know, the results obtained are more formal. Nevertheless, let us start with the 0th order formal diagonalization. Starting with the Hamiltonian of an electron in a periodic potential plus an external perturbation

$$H_0(\mathbf{P},\mathbf{R}) = \frac{\mathbf{P}^2}{2m} + V(\mathbf{R}) + v(\mathbf{R}) \tag{41}$$

with $v(\mathbf{R}) = \mathbf{E}.\mathbf{R}$ and $\mathbf{E}(t)$ a time dependent electric field, the zeroth order diagonalization can be done formally with a $\mathbf{K}$ dependent unitary matrix $U_\alpha(\mathbf{K})$, where $\mathbf{K}$ is the pseudo-momentum of the Bloch bands [6] [5]. Therefore, only the position acquires a Berry phase, i.e., $\mathcal{A}_\alpha^R(\mathbf{K}) = i[U\nabla_P U^+]^+$ and $\mathcal{A}_\alpha^P = -i[U\nabla_R U^+]^+ = 0 + O(\alpha)$ implying $\mathcal{A}_\alpha^{P_l,R_l} = 0 + O(\alpha)$.

As a consequence, the diagonalized Hamiltonian $\varepsilon_\alpha(\mathbf{K},\mathbf{R})$ at order α, projected on a particular band of index n is given by :

$$\varepsilon_{\alpha,n}(\mathbf{K},\mathbf{r}_n) = \widetilde{\varepsilon}_n(\mathbf{K}) + v(\mathbf{r}_n) \tag{42}$$

where $\widetilde{\varepsilon}_n(\mathbf{K})$ is the energy of the unperturbed nth band (i.e. when $v(\mathbf{R}) = 0$) and $\mathbf{r}_n$ the covariant position operator defined as the projection of $\mathbf{R} + \alpha\mathcal{A}_\alpha^R$ on the nth band:

$$\mathbf{r}_n = \mathbf{R} + \alpha\mathcal{A}_{n,\alpha}^R(\mathbf{K}) \tag{43}$$

where $\mathcal{A}^R_{\alpha,n}$ is the projection of the matrix $\mathcal{A}^R_\alpha$ on the nth band. The equations of motion are easily deduced to be

$$\dot{\mathbf{r}}_n = \nabla_{\mathbf{K}}\varepsilon_{\alpha,n} + \frac{1}{\hbar}\dot{\mathbf{K}}\times\Theta^{rr}_n$$
$$\dot{\mathbf{K}} = \nabla_{\mathbf{r}}\varepsilon_{\alpha,n} = \mathbf{E} \tag{44}$$

with the Berry curvature defined as $[r_{n,i}, r_{n,j}] = \Theta^{rr}_{n,ij} = \partial_i\mathcal{A}^R_{n,\alpha} - \partial_j\mathcal{A}^R_{n,\alpha}$. The second term in Eq. 44 is called the anomalous velocity and it is was shown to drive important new effects, such as the discovery of a monopole in momentum contribution to the conductivity of Bloch electrons in particular materials [16]. It is then interesting to check if this equation is changed beyond the semiclassical level.

2. Second Order and more

The computation of the energy to the second order needs the value of the transformation matrix at the first order in α. Consider therefore the 0th order differential equations for the transformation matrix Eq. 17

$$0 = \left[\partial_\alpha U_\alpha\left(\mathbf{K},\mathbf{R}\right)U^+_\alpha\left(\mathbf{K},\mathbf{R}\right),\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\right]^- + \frac{1}{2}\left[\mathcal{A}^{R_l}_\alpha\nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right) + \nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\mathcal{A}^{R_l}_\alpha\right]^- \tag{45}$$

and Eq. 18

$$0 = \partial_\alpha U_\alpha(\mathbf{K},\mathbf{R})U^+_\alpha(\mathbf{K},\mathbf{R}) + U_\alpha(\mathbf{K},\mathbf{R})\partial_\alpha U^+_\alpha(\mathbf{K},\mathbf{R}) \tag{46}$$

We see that nothing ensures that: $\left[\mathcal{A}^{R_l}_\alpha\nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right) + \nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\mathcal{A}^{R_l}_\alpha\right]^- = 0$. To solve for the transformation matrix, we proceed as for the photon and decompose at the first order $U_\alpha(\mathbf{K},\mathbf{R}) = U_0(\mathbf{K},\mathbf{R}) + \alpha U_1(\mathbf{K},\mathbf{R})$, so that, taking into account the specific form of $v(\mathbf{R})$ our equations Eqs. 45 and 46 reduce to

$$\left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R}), \varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\right] = -\left[\mathcal{A}^{R_l}_\alpha, E_l\right]^-$$
$$U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R}) + U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R}) = 0$$

Introducing the band indices, one easily sees that these two equations reduce to the $2n^2 - n$ following independent equations for $2n^2$ real variables (n, the number of bands can of course be infinite; this does not invalidate the argument)

$$\left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})\right]_{mn}\left(\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)_n - \varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)_m\right) = -\left[\mathcal{A}^{R_l}_\alpha, E_l\right]_{mn}, \text{ for } m < n$$
$$\left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})\right]_{mn} + \left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})\right]_{mn} = 0$$

Once again, we are left with a gauge choice on the diagonal. We can simply impose as a condition that the diagonal elements are null. Actually, our equation imposes that $\left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})\right]_{nn}$ is an imaginary number. As a consequence, similarly to the photon, composing $U_\alpha(\mathbf{K},\mathbf{R})$ on the left with the unitary matrix X defined by

$$X_{mn} = 1 - \alpha\delta_{mn}\left[U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})\right]_{nn} \tag{47}$$

yields a diagonalization matrix with zero on the diagonal.

Having chosen the gauge, the equations for $U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})$ can be solved formally, through the Cramer rules. Fortunately, given our very simple case of potential, we get

$$\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)_n - \varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)_m = \tilde{\varepsilon}_\alpha\left(\mathbf{K}\right)_n - \tilde{\varepsilon}_\alpha\left(\mathbf{K}\right)_m \tag{48}$$

which does not depend on $\mathbf{R}$. As a consequence, $U_1(\mathbf{K},\mathbf{R})U^+_0(\mathbf{K},\mathbf{R})$ and thus $U_1(\mathbf{K},\mathbf{R})$ is only a function of $\mathbf{K}$.

We can thus write

$$U_\alpha(\mathbf{K},\mathbf{R}) = U_0(\mathbf{K}) + \alpha U_1(\mathbf{K}) \tag{49}$$

As a consequence at the first order we will have again.:

$$\mathcal{A}^R_\alpha = i\left[U_\alpha\nabla_K U^+_\alpha\right]^+ + O\left(\alpha^2\right) \tag{50}$$

and for the other Berry curvatures we have $\mathcal{A}^P_\alpha = 0 + O\left(\alpha^2\right)$, and $\mathcal{A}^{P_l,R_l}_\alpha = 0 + O\left(\alpha^2\right)$. Let us just mention that the Berry phase in R is now different from its the zeroth order value. It has now a term proportional to α which is included in its definition.

Consider now the differential equation for the energy at the first order in α. A simplification arise, since here, at the first order

$$Asym\left\{\nabla_{P_l}\nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\right\} - U_\alpha Asym\left\{\nabla_{P_l}\nabla_{R_l}H_0\left(\mathbf{P},\mathbf{R}\right)\right\}U_\alpha^+ = 0 \tag{51}$$

actually $\mathbf{K}$ and $\mathbf{R}$ are not mixed in ε_α or H_0. As a consequence, and given our previous results, the projection of our equation on the diagonal part leads to

$$\frac{d}{d\alpha}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right) = \frac{1}{2}\left[\mathcal{A}_\alpha^{R_l}\nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right) + \nabla_{R_l}\varepsilon_\alpha\left(\mathbf{K},\mathbf{R}\right)\mathcal{A}_\alpha^{R_l}\right]^+ \tag{52}$$

Exactly as in the photon case, this equation has the second order solution after projection on the nth band

$$\varepsilon_{\alpha,n}\left(\mathbf{K},\mathbf{r}_n\right) = \tilde{\varepsilon}_n(\mathbf{K}) + v\left(\mathbf{r}_n\right) \tag{53}$$

where now $\mathbf{r}_n = \mathbf{R} + \alpha\mathcal{A}_{\alpha,n}^R$. Note that $\alpha\mathcal{A}_{\alpha,n}^R$ is actually of order α^2. Therefore the energy has formally the same expression than in the first order case. The only difference stems from the potential energy because the position operator get a α^2 contribution through the presence of the Berry connection.

As a consequence, the equations of motion are formally the same as for the first order (removing the band index), i.e.,

$$\dot{\mathbf{r}}_n = \nabla_{\mathbf{K}}\varepsilon_{\alpha,n} + \frac{1}{\hbar}\,\overset{\bullet}{\mathbf{K}}\times\Theta_n^{rr}$$

$$\overset{\bullet}{\mathbf{K}} = \nabla_{\mathbf{r}_n}\varepsilon_{\alpha,n} = \mathbf{E}$$

The only difference with respect to the semiclassical equations of motion Eq.44 is that the Berry connection gets a contribution of order $\hbar^2$ but formally the equations of motion are unchanged.

To conclude this section let us state the following important result. One can easily check that all our construction can be generalized to all orders in $\hbar$. As a consequence, the Hamiltonian form for $\varepsilon_{\alpha,n}\left(\mathbf{K},\mathbf{r}_n\right)$ is valid to all orders, and the equation of motions are in fact quantum operator equations. The only difference appearing when diagonalizing recursively, consists in new contributions to the Berry connection.

This is a important new result, because these equations were considered until now has semiclassical equation of motion with the usual restrictions imposed in this case. It would be interesting to check if this result is generalizable to spatially variable electric field and in the presence of a magnetic field, but then the equations get quickly cumbersome.

V. CONCLUSION

Some recent applications of semi classical methods to several branches of Physics, such as spintronics or solid state physics have shown the relevance of Berry Phases contributions to the dynamics of a system, leading notably to the discovery of the intrinsic spin Hall effect. However, these progresses called for a rigorous Hamiltonian treatment that would allow for deriving naturally the role of the Berry phase in theses systems and to go beyond the semiclassical level. In this paper, we presented a new diagonalization method for a generic matrix valued Hamiltonian, based on a formal expansion in power of $\hbar$. A differential equation connecting two diagonalization processes for two very close values of $\hbar$, considered as a running parameter, was derived. The integration of this differential equation allows the recursive determination of the series expansion of the diagonalized Hamiltonian in powers of $\hbar$. This approach, which results in effective Hamiltonians with Berry phase corrections, goes beyond previous works on the semiclassical diagonalization of quantum Hamiltonians. The resulting generic equations of motion are also corrected by Berry phase terms of higher order in $\hbar$. As physical applications, we considered a spinning massless particle propagating in a isotropic inhomogeneous medium and showed that both the energy and the velocity get quantum corrections of order $\hbar^2$. We also derived formally to all order in $\hbar$ the energy spectrum and the equations of motion of Bloch electrons in an external constant electric field, showing that the equations of motion are actually quantum operator equations (valid to each order in $\hbar$). It would be interesting to check if this result persists for variable electric fields and in the presence of magnetic fields. Our approach is a general one and will be applied in the future to other condensed matter systems as well as in particle physics.

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